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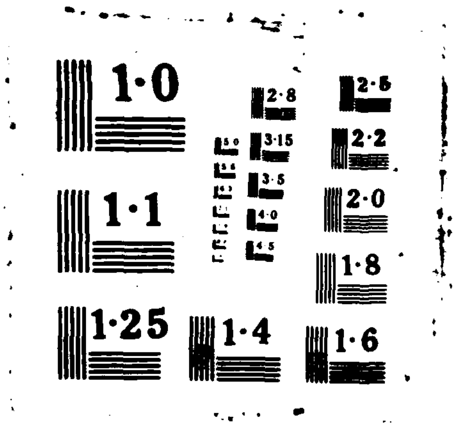
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FINAL REPORT

AMG: BASIC DEVELOPMENT, APPLICATIONS AND THEORY

distribution unlimited.

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Final Report: AMG: Basic Development, Applications and Theory

I. Introduction

The central focus was the study of algebraic multigrid (AMG), which was in fact developed under this project. Since most of the papers previously submitted to AFOSR included a description of AMG and the major results of the project, only a brief overview will be given here.

Conventional or geometric multigrid algorithms depend on knowledge of the underlying geometry for a given problem (e.g., a partial differential equation). This knowledge is used to predetermine coarser grids and the attendant operators and intergrid transfers. Although very efficient solvers can be developed in this way, the dissemination and use of geometric multigrid have been impeded by the need to tailor the algorithm to each application. A fairly general "black box" solver based on multigrid principles would be useful in overcoming these difficulties and promoting multigrid applications.

Algebraic multigrid uses no explicit knowledge of an underlying geometry to produce coarser levels. In fact, only the matrix entries and a few algorithm parameters are used to determine the coarser levels and the remaining multigrid processes. The motive is to maintain the typical multigrid efficiency by determining coarser levels that properly reflect the errors that relaxation cannot effectively reduce.

For certain classes of matrices (e.g., symmetric positive-type), the means for obtaining this motive is relatively easy to describe: It can be shown (B2) that point Gauss-Seidel for such matrices achieves (algebraic) smoothness in the sense that the errors after just a few sweeps are "locally constant", that is, variables that are strongly coupled via large off-diagonal matrix entries must exhibit similar errors in the approximate solution. The coarsening process may therefore use a Ritz-type variational formulation in an attempt to approximate such errors, that is, it is enough to determine an interpolation process that ensures that such errors are in the range of interpolation. This approximation property must be achieved while maintaining low complexity of the resulting coarse level problems. This can generally be accomplished by p-point interpolation which is an efficient way of ensuring that each variable that does not become a coarse level variable is strongly dependent on approximately p that are. The means for implementing this process are quite complicated (B3), but the principles are straightforward. Moreover, sharp

convergence rates can be proved in this case and in more general cases, including block positive-type matrices such as those that arise from discretizing Stokes's equations (cf. (B2)).

The main difficulty in applying AMG to new classes of matrices is one of determining the sense of smoothness (of relaxed errors) for these classes. Once this sense is determined, efficient coarse-to-fine interpolations can be devised. Automatic ways for computationally detecting the sense of smoothness from preliminary relaxation sweeps are one of the main objectives of the proposed research. Such methods are expected to enhance the AMG efficiency even for classes where it is already successfully applied.

AMG should not be viewed as a way to completely eliminate the need to carefully consider each application. It will never be a complete black box solver in the sense that it will work efficiently over all symmetric positive definite matrices, say. No method does. But it can become a significant computational tool that will significantly reduce the design effort for multigrid applications. It should also lead to a better understanding of the multigrid processes themselves and provide guidance in the coarsening process for new applications.

AMG shows much promise. During the project, it was in fact applied to a wide variety of essentially positive-type problems, including anisotropic and ill-behaved diffusion equations as well as certain nonsymmetric problems, especially convection dominated diffusion equations, and some purely algebraic problems that arise in geodesy, with extension to a broader class of problems, applications, and software development. The following sections will briefly discuss only the broader areas of progress made during the project.

II. Areas of Progress

The objective of this project was the systematic development and analysis of algebraic multigrid methods for solving partial differential boundary value problems. This began gradually, continuing the progression from simpler problems to more difficult ones, introducing each complexity in its turn, and studying first each difficulty in isolation from others. (Application-oriented multigrid studies have too often started with too complicated a problem and have as a result failed to realize some of the crucial algorithmic features.)

1. Basic AMG Development

The basic efforts of algorithm development are categorized as follows:

a. Symmetry. The project team developed a fully automatic AMG (B3) for treating essentially positive-type symmetric matrices (matrices with the property that their dominant part has nonpositive off-diagonal entries and nonnegative row sums).

Another direction of the current project, which is relevant even to positive-type cases, was the study of methods for obtaining enhanced interpolation accuracy. To be specific, even though an algebraic sense of smoothness is known (B2, Sec. 3.5), it may be fairly crude so that the effective order of interpolation is too low (cf. the example in (B2, Sec. 4.7)). Although the W-cycle rates are reasonable even for such cases, it is important to attempt to achieve a better sense of smoothing here. Prerelaxation methods were developed for this purpose. The basic idea of this approach is to perform a few relaxation sweeps on several initial approximations of the homogeneous system in order to obtain a representative set of vectors that exhibit smoothness. These vectors can then be easily examined to determine the common relationships between components of smooth vectors and to provide a basis for determining interpolation.

Another objective in the study of symmetric problems was the treatment of the more general class of locally positive definite (B2) matrices. For such matrices that are not essentially block positive-type, a crude sense of smoothness can be determined from the explicit local form that characterizes this class (B2, Sec 3.5). Yet this form is not always explicitly available and, even when it is, may not be explicit for the coarser level matrices. The simplest example for this situation is a general M matrix where the scaling needed to convert it to positive-type is not explicitly given. The first step here was, therefore, to apply AMG to such an M-matrix, A. This was done using a simple prerelaxation scheme of the above type. In this case the "smoothing relations" that the prerelaxation provided are equivalent to approximately finding the relative scalings (i.e., the approximate ratios between the entries of the positive diagonal matrix D for which DAD is positive-type). This was achieved to the degree that is needed by just a few relaxation sweeps on the homogeneous system with an initial guess related to the diagonal of A.

b. Nonsymmetry. Experiments with nonsymmetric matrices focused on determining how far the "symmetric" version of AMG could be carried. Basing the process entirely on the rows of the matrix, the experiments in (S1) for singular perturbation problems showed that AMG maintains efficiency so long as the dominance of convection terms is not so large that there is a total loss of positive-type. In typical physical problems, this means that the (artificial) viscosity terms should be of a size that is typical in upstream differencing.

2. Applications

It was essential for both focus and relevance and for guiding algorithm development that the project be driven by a specific set of increasingly difficult but realistic application problems. AMG has thus far been studied in the context of two and three dimensional diffusion and diffusion-convection problems and (originally discrete) geodetic problems, but the project began a progression into increasingly more complicated equations. Following is a short summary of the problems beyond the present applications that were initial objects of study.

a. Structural Analysis. The project began to apply AMG to the linear equations and eigenvalue problems that arise in discretizing, respectively, static and dynamic structural analysis equations. This was done by using AMG as a linear solver in existing structures codes.

b. Stokes Equations. Initial tests of AMG began on the symmetric Stokes equations.

c. Navier-Stokes and Euler Equations. Early consideration was also given to applying MAG to Navier-Stokes and Euler equations.

d. Vectorization. The project has access to a Cyber 205 vector computer. Recent developments include fully vectorized codes for both a model Poisson solver (BA1) and a 3-d diffusion equation solver (G1) based on conventional multigrid. The impressive efficiency exhibited by these codes cannot be expected to be fully achieved by AMG, but it was nevertheless important to study the vectorizability of AMG processes. Initial study began by considering the use of geometric information to develop logically regular grids. This was a first step in the direction of AMG vectorization.

3. Theory

The development of new theoretical tools and insights proved indispensible during the past evolution of AMG. The need for precise quantitative insights,

realistically dependent on the various algorithmic parameters, and the fact that the traditional local mode analysis is not applicable to general AMG, was motivation for development of new theoretical approaches (B2), which, incidentally, provided improved rigorous foundation even for traditional (geometric) multigrid.

The first step will be to complete the theory for the symmetric case, as outlined in (B2, Sec. 1), with additional studies related to new algorithmic developments such as the automatic calculation of smoothing relations.

Initial study considered the extension of the symmetric theory (B2) to nonsymmetric matrices.

Another theoretical direction that was pursued involved the establishment of a theory based on C - F relaxation (B3). The theory thus far does not take into account any special ordering of the relaxation process, yet numerical experience with AMG suggests that relaxing first on the coarse grid (C) points followed by that on the remaining (F) points is often more effective. Some results for C - F relaxation were in fact achieved by viewing AMG as approximate total reduction.

Stephen F. McCormick, Ph.D.
Principal Investigator

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